

Abstract No. nuck466

Polarization-dependent Electronic Structure of AlB_2 Single Crystals

N. Nücker, S. Schuppler, R. Heid, K.-P. Bohnen, Th. Wolf (Forschungszentrum Karlsruhe, Germany), T. Mizokawa (U of Tokyo, Japan), M. Merz (RWTH Aachen, Germany), D. Arena, J. Dvorak, Y.U. Idzerda (Montana State U.)

Beamline(s): U4B

Introduction: AlB_2 is a compound isostructural to the new 40K superconductor MgB_2 with its hexagonal, layered crystal structure. Knowledge of its electronic structure as well would form an important basis for understanding future, similarly detailed studies on MgB_2 .

Methods and Materials: High-quality single crystals were studied with polarization-dependent near-edge x-ray absorption fine structure (NEXAFS) at the boron 1s edge, giving information on the unoccupied electronic structure with B 2p character and its orbital characteristics. Energy-dispersive fluorescence-yield (EDFY) detection with an array of Si(Li) semiconductor detectors was employed to ensure bulk sensitivity and to effectively suppress possibly energy-dependent contributions from other edges.

Results: The B 1s NEXAFS exhibit a strong anisotropy between spectra for in-plane polarization and spectra for polarization perpendicular to the plane [1], giving considerably more information than previous studies on polycrystalline material [2]. For example, close to the onset at the Fermi level E_F the observed in-plane absorption is strongly suppressed – by about a factor of 10 – compared to the out-of-plane absorption, which shows a sharp Fermi cutoff. Only several eV above onset the in-plane absorption has caught up. This appears like a counter-intuitive observation as the layered crystal structure seems to suggest, at first glance, the opposite behavior.

We also performed LDA band-structure calculations with mixed-basis pseudopotentials for AlB_2 and find excellent agreement of all major NEXAFS structures, both for in-plane and out-of-plane polarization, with the projected band structure of B 2p character. The strikingly strong anisotropy at E_F observed in NEXAFS is extremely well reproduced in the theoretical results.

On a more technical note, this study clearly demonstrates the feasibility of EDFY-NEXAFS even for such ultralow fluorescence energies (~ 180 eV), allowing the user to carry over the well-known advantages of FY detection to the study of these exotic materials. To our knowledge, this is the first polarization-dependent EDFY-NEXAFS study on the B 1s edge of a single-crystalline compound.

Acknowledgments: We gratefully acknowledge continuous and valuable support by NSLS staff, in particular G. Nintzel and S. L. Hulbert.

References:

[1] N. Nücker *et al.*, to be published.

[2] T. A. Callcott *et al.*, Phys. Rev. B **64**, 132504 (2001); N. Nakamura *et al.*, Phys. Rev. B **64**, 174504 (2001).